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Isothermal compressibility in binary platinum based melts

I G Kosnureva[1], M A Spiridonov[1], M M Mitko[2] and V P Chentsov[2]

[1]Urals State Technical University-UPI, Mira 19, Ekaterinburg, 620002, Russia

E-mail: sma@mtf.ustu.ru

[2] Institute of Metallurgy of Urals Division, Russian Academy of Sciences

Abstract. The method based on concentration dependences of density and formation heat values for determination of fluctuation structure factors and isothermal compressibility has been used for binary Pt-Si and Pt-Sn melts.

1. Introduction

The partial structure factors values in low angle (thermodynamic) limit are necessary for definition of the effective atomic potentials in non-crystalline materials and calculation of specific electrical conductivity in the Faber-Ziman theory. Direct determination of the structure factors (SF) at small angles in diffraction experiments is difficult enough due to initial beam masking action and low ratio of useful signal to the background noise, especially at a high temperature. At the same time the extensive experimental material on density and formation heat of binary melts permitting to prognosticate fluctuation structure factor values, especially in the hardly accessible for diffraction investigations area, is accumulated now.

2. Theoretical background

The method is based on the equation, connecting the partial structure factors in low angle limit with the average atomic density ρ_0 and isothermal compressibility β_T. In particularly, for a binary systems the limits of a_{ij} (Ashcroft-Langreth's) and a_{xx}(Thornton-Bhatia's) fluctuation correlation SF is known [1]:

$$a(0) = \rho_0 \, k \, T \, \beta_T = \lim_{q \to 0} \frac{a_{11} \, a_{12} - a_{12}^2}{a_{xx} \, /[\, x \, (1 - x)]}, \qquad (1)$$

where $q = 4 \sin\theta / \lambda$, θ is a half of scattering angle, λ is the wave length and x is atomic concentration.

Using the relations between the different sets of partial SF [1]

$$a_{11} = (1 - x) \, a(0) + [(1 - x)\delta^2 + \frac{1}{1 - x} - 2\delta] \, a_{xx}(0), \qquad (2)$$

$$a_{22} = x \, a(0) + [x\delta^2 + 2\delta + \frac{1}{x}] \, a_{xx}(0), \qquad (3)$$

$$a_{12}=\left[x(1-x)\right]^{0,5}a(0)+\left\{\left[x(1-x)\right]^{0,5}\delta^2+\left[\left(\frac{1-x}{x}\right)^{0,5}\left(\frac{x}{1-x}\right)^{0,5}\right]\delta-\left[\frac{1}{x(1-x)}\right]^{0,5}\right\}a_{xx}(0), \quad (4)$$

adding expressions for the total SF [2]:

$$a(q)=\frac{1}{<f(q)^2>}\left\{<f(q)>^2 a_{nn}(q)+2\Delta f(q)<f(q)>a_{nx}(q)+<\Delta f(q)>^2 a_{xx}(q)\right\}, \quad (5)$$

and for Flory's model [3]:

$$\Delta H_f = RT\,\frac{(\beta-1)^3}{2\beta\delta^3}\left[1+x(1-x)\,\delta^2-\frac{x(1-x)}{a_{xx}(0,x)}\right] \quad (6)$$

where $<f(q)^2> = \sum x_i f_i(q)$, $\Delta f(q) = |f_1(q) - f_2(q)|$, $f_i(q)$ is atomic scattering factors, $\beta = \frac{\bar{V}_1}{\bar{V}_2} \le 1$,

δ is dilatometric factor equal to

$$\delta = \frac{1}{V}\left(\frac{\partial V}{\partial x}\right)_{p,T,N} = \frac{\bar{V}_1 - \bar{V}_2}{x\bar{V}_1 + (1-x)\bar{V}_2},$$

and $\bar{V}_1, \bar{V}_2$ are partial molar volumes of the components, we shall receive the system of equations [4] with the corresponding number of unknown variables (i = 1,2...5):

$$Y_i = 0, \quad (7)$$

where

$$Y_1 = a_{11} - (1-x)\,a(0) - Z_{11}\,a_{xx}, \quad (8)$$

$$Y_2 = a_{22} - x\,a(0) - Z_{22}\,a_{xx}, \quad (9)$$

$$Y_3 = a_{12} - [x(1-x)]^{1/2}\,a(0) - Z_{12}\,a_{xx}, \quad (10)$$

$$Y_4 = a(0) - [a_{11}a_1 - a_{12}^2] / (a_{xx}/x(1-x)), \quad (11)$$

$$Y_5 = a_{xx} - x(1-x) / \{1 + x(1-x)\,\delta^2 - 2\,\Delta H_f\,\beta\,\delta^3/[RT(\beta-1)^3]\}. \quad (12)$$

Here, for a compact presentation, Z_{11}, Z_{22} and Z_{12} coefficients in (8)-(10) denote:

$$Z_{11} = (1-x)\,\delta^2 + 1/(1-x) - 2\,\delta, \quad (13)$$

$$Z_{22} = x\,\delta^2 + 1/x + 2\,\delta, \quad (14)$$

$$Z_{12} = [x(1-x)]^{1/2}\,\delta^2 + \{[1-x)/x]^{1/2} - [x/(1-x)]^{1/2}\}\,\delta - 1/(1-x)^{1/2}. \quad (15)$$

3. Results of calculations

The above approach for fluctuation SF and isothermal compressibility calculation using the experimental data for formation heat and density of melts was applied for Pt-Si and Pt-Sn systems. The obtained results are shown in the Figure 1 and Table 1.

4. Acknowledgements

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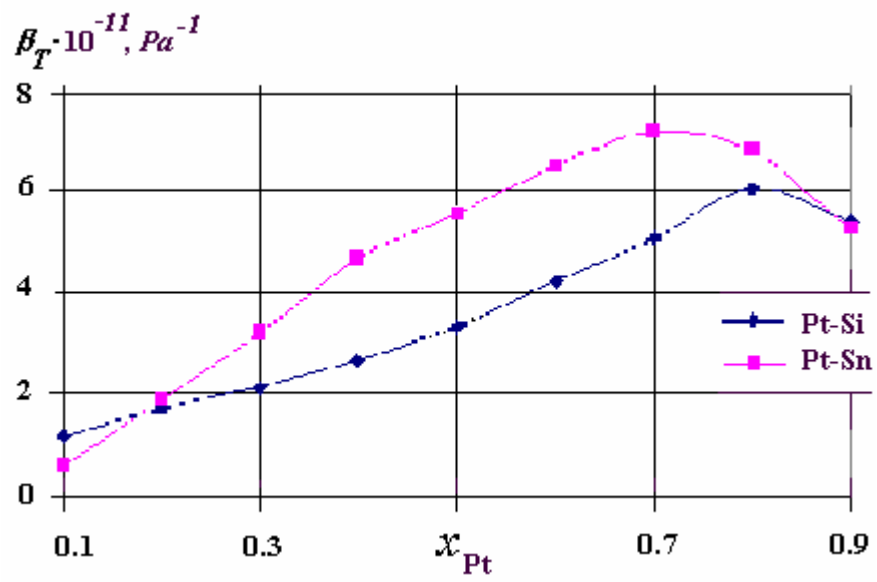

Figure 1. The concentration dependencies of isothermal compressibility for binary platinum based melts.

Table. The fluctuation structure factors in low angle limit and isothermal compressibilities of binary melts including Pt at T=2073 K

$x_{Si(Sn)}$	$-\delta$	$a_{xx}\,10^2$	$a_{nx}\,10^3$	$a_{nn}\,10^2$	$a(0)\,10^2$	$\beta_T\,10^{11}$, Pa^{-1}
						Pt-Si
0.1	0.02	5.56	1.11	6.50	12.70	5.4
0.2	0.03	5.49	1.66	10.00	12.50	6.1
0.3	0.08	4.25	3.49	8.25	9.93	5.1
0.4	0.14	3.44	4.72	6.84	8.18	4.2
0.5	0.19	2.68	4.99	5.46	5.26	3.3
0.6	0.21	2.13	4.57	4.45	5.31	2.6
0.7	0.24	1.72	4.09	3.63	4.36	2.1
0.8	0.24	1.48	3.61	3.01	3.66	1.7
0.9	0.25	1.09	2.73	2.06	2.54	1.1
						Pt-Sn
0.1	0.19	4.59	0.89	7.48	7.52	5.2
0.2	0.28	5.36	1.49	9.54	9.59	6.8
0.3	0.44	5.12	2.20	10.10	10.21	7.2
0.4	0.60	4.27	2.57	9.76	9.86	6.5
0.5	0.76	3.70	2.81	9.57	9.67	5.6
0.6	0.94	3.05	2.86	9.44	9.54	4.6
0.7	1.18	2.18	2.58	8.37	8.43	3.2
0.8	1.49	1.41	2.09	6.86	6.82	1.9
0.9	1.91	0.78	1.49	5.34	4.13	0.5

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